REFERENCES

Agatonovic S, Beresford R, Yusof P. ANN modeling of the penetration across a polydimethylsiloxane membrane from theoretically derived molecular descriptors. J Pharm Biomed Anal. 2001; 26(2): 241-254.

Bharath E, Manjula S, Vijaychand A. *In silico* drug designtool for overcoming the innovation deficit in the drug discovery process. Int J Pharmacy and Pharml Sci. 2011; 3(2): 8-12.

Chandrasekar D, Jaymin S, Senapati S and Uday K. Prediction of Vitreal Half-Life based on drug physicochemical properties: Quantitative Structure-Pharmacokinetic relationships (QSPKR). Pharmceut Res. 2009; 26(5): 1236-1260.

Chen Y, Cameron K, Guzman-Perez A, Perry D, Li D, Gao H. Structure pharmacokinetic relationship of *in vivo* rat biliary excretion. Biopharm Drug Disposition. 2010; 31(1): 82-90.

Cheng D, Xu R, Liu C X. Relationship of quantitative structure and pharmacokinetics in fluoroquinolone antibacterials. W J Gastroenterol. 2007; 13(17): 2496-2503.

Chohan KK, Paine SW, Water NJ. Advancements in predictive *in silico* models for ADME. Current Chemical Biology. 2008; 2: 215-228.

Cupid C, Beddell R, Lindon C, Wilson D, Nicholson K. Quantitative structure-metabolism relationships for substituted benzoic acids in the rabbit: prediction of urinary excretion of glycine and glucuronide conjugates. Xenobiotica. 1996; 26(2): 157-176.

Ekins S, Waller C, Swaan P, Cruciani G, Wrighton S, Wikel J. Progress in predicting human ADME parameters in silico. J Pharmacol Toxicol Methods. 2000; 44(1): 251-272.

Estrada E, Uriarte E, Molina E, Simon- Manso Y, Milne GWA. An Integrated in Silico Analysis of Drug-Binding to Human Serum Albumin. J. Chem. Inf. Model. 2006; 46: 2709-2724.

Gandhi Y, Morris M. Re-evaluation of a Quantitative Structure Pharmacokinetic Model for Biliary Excretion in Rats. DMD Fast Forward.2012: 1-18.

Ghafourian T, Jalali M, Dastmalchi S, Khorasani T, Hakimiha N, Nokhodchi A. QSPR models for the prediction of apparent volume of distribution. Int J Pharm. 2006; 319(1-2): 82-97.

Gombar V, Silver I, Zhao Z. Role of ADME characteristics in drug discovery and their *In Silico* evaluation: *In Silico* screening of chemicals for their metabolic stability. Curr Top Med Chem. 2003; 3(11): 1205-25.

Grabowski T, Jaroszewski J, Gad S, Feder M. Correlation Between *In Silico* physicochemical Characteristics of Drugs and Their Mean Residence Time in Human and Dog. 2012.

Grover M, Singh B, Bakshi M. Quantitative structure-property relationships in pharmaceutical research - Part 1. Pharm Sci Technolo Today. 2000; 3(1): 28-35.

Hasegawa K, Shindoh H, Shiratori Y, Ohtsuka T, Aoki Y, Ichihara S, Horii I, Shimma N. Cassette dosing approach and quantitative structure-pharmacokinetic relationship study of antifungal N-myristoyltransferase inhibitors. J Chem Inf Comput Sci. 2002; 42(4): 968-975.

Herman A, Vengpedersen P. Quantitative structure-pharmacokinetic relationships for systemic drug distribution kinetics not confined to a congeneric series. J Pharm Sci. 1994; 83(3): 423-428.

Karalis V, Kakoulidou A, Macheras P. Quantitative structure-pharmacokinetic relationships for disposition parameters of cephalosporins. Eur J Pharm Sci. 2003; 20(1): 115-123.

Katritzky R,FaraC, Karelson M.QSPR of 3-aryloxazolidin-2-one antibacterials. Bioorg Med Chem. 2004; 12(11): 3027-3035.

Kumar A, Singh S, Jain S, Kumar P. SYNTHESIS, Antimicrobial evaluation, qsar and *in silico* admet studies of decanoic acid derivatives. Acta Poloniae Pharmaceutica - Drug Research. 2011; 68: 191-204.

Laznicek M. Renal clearance-lipophilicity relationships of some organic acids in rabbits, rats and mice. J Pharm Pharmacol. 1992; 44(3): 255-257.

Linnankoski J, Makela M, Ranta P, Urtti A, Yliperttula M. Computational prediction of oral drug absorption based on absorption rate constants in humans. J Med Chem. 2006; 49(12): 3674-3681.

Lipscomb JC, Meek ME, Krishnan K, Kedderis KL, Clewell H, Haber L. Incorporation of pharmacokinetic and pharmacodynamic data into risk assessments. Society of Toxicology. 2002: 1-25.

Louis B and Agrawal VK. Quantitative structure-pharmacokinetic relationship (QSPkR) analysis of the volume of distribution values of anti-infective agents from J group of the ATC classification in humans. Acta Pharma. 2012; 62: 305-323.

Mager E, Jusko J. Quantitative structure-pharmacokinetic/pharmacodynamic relationships of corticosteroids in man. J Pharm Sci. 2002; 91(11): 2441-51.

Marechal E. Chemogenomics: a discipline at the crossroad of high throughput technologies, biomarker research, combinatorial

chemistry, genomics, cheminformatics, bioinformatics and artificial intelligence. Comb Chem High Throughput Screen. 2008; 11(8): 583-586.

Mayer M, VandewaterbeemdH. Development of quantitative structure-pharmacokinetic relationships. Environ Health Perspect. 1985; 61: 295-306.

Paul Y, Parina, Singla A, Singh B. *In Silico* Quantitative structure pharmacokinetic relationship modeling on antidiabetic drugs: Half-Life Int. J. Chem. Sci : 2013; 11(1) : 177-185.

Paul Y, Dhake S, Parle M, Singh B. *In Silico* Quantitative Structure Pharmacokinetic Relationships for Quinolone Drugs: Biological Half-Life. Asian J Chem. 2010; 22(6): 4880-4890.

Paul Y, Dhake S, Parle M, Singh B. Quantitative structure pharmacokinetic relationship studies for drug clearance of quinolone drugs. Res J Pharm Tech. 2008; 1(2): 106-111.

Paul Y, Parina, Singla A, Singh B. *In Silico* Quantitative structure pharmacokinetic relationship modeling on antidiabetic drugs: Serum Protein Binding. Internationale Pharmaceutica Sciencia. 2012; 2(4): 39-43.

Paul Y, Parle M, Dhake S, Singh B. *In Silico* Quantitative Structure Pharmacokinetic Relationships for Elimination Half-Life of Fluoroquinolones. Asian J Chem. 2009; 21(7): 5483-5487.

Radouane A, Pehourcq F, Tramu G, Creppy E and Bannwarth B. Influence of lipophilicity on the diffusion of cephalosporins into the cerebrospinal fluid. Fund ClinPharmaco. 1996, 10(3): 309-313.

Rochani AK, Suma BV, Kumar S, Jays J, Madhavan V. QSAR, ADME and QSTR studies of some synthesized anti-cancer 2-indolinone derivatives. Int J Pharm Bio Sci. 2010; 1(4): 208-218.

Rodrigues CR, Leal B, Oliveira KN, Castro HC. *In vitro* and *in silico* Approaches to the Identification of New Compounds with Antibacterial Profile. Systemics Cybernetics Informatics. 2013; 11: 62-65.

Seedher N, Bhatia S, Singh B, Quantitative Correlation between Theoretical Molecular Descriptors and Drug-HSA Binding Affinities for Various Cox-2 Inhibitors. Chem Biol Drug Des. 2008, 72:297-302.

Seedher N. Quantitative structure protein binding relationships for some non-steroidal antiinflammatory drugs. Ind J Pharm Sci. 2000; 62(5): 402-404.

Seydel K. Quantitative structure-pharmacokinetics relationships and their importance in drug design, possibilities and limitations. Methods Find Exp Clin Pharmacol. 1984; 6(10): 571-581.

Singh B, Singla A, Paul Y, Sehgal R. Clinical research in India: Retrospects and Prospects. Pharm Rev. 2010: 39 - 46.

Singh SK, Saini S, Verma B, Mishra DN. Quantitative structure pharmacokinetic relationship using artificial neural network: A review. Int J Pharm Sci Drug Res. 2009; 1(3): 144-153.

Singla A, Singh B, Paul Y. *In silico* quantitative structure pharmacokinetic relationship modeling on aryl carboxylic acid: Volume of distribution and serum protein binding. Int J Chem Sci. 2012; 10(1): 547-593.

Turner V, Maddalena J, Cutler J, Kustrin S. Multiple pharmacokinetic parameter prediction for a series of cephalosporins. J Pharm Sci. 2003; 92(3): 552-559.

Turner V, Maddalena J, Cutler J. Pharmacokinetic parameter prediction from drug structure using artificial neural networks. Int J Pharm. 2004; 270(1-2): 209-219.

Vandergraaf H, Nilsson J, Vanschaick A. Danhof M. Multivariate quantitative structure-pharmacokinetic relationships (QSPKR) analysis of adenosine A1 receptor agonists in rat. Pharm Sci. 1999; 88(3).

Venkataramana CHS, Sravani KMR, Singh SS, Madhavan V. *In-silico* ADME and toxcity studies of some novel indole derivatives. J Applied Pharm Sci. 2011; 01 (10): 159-162.

Verma M, Chaudhry A, Fahrni C. Predicting the photoinduced electron transfer thermodynamics in polyfluorinated 1,3,5-triarylpyrazolines based on multiple linear free energy relationships. Org Biomol Chem. 2009; 7(8): 1536-1546.

Yamada Y, Ito K, Nakamura K, Sawada Y, Iga T. Prediction of therapeutic doses of beta-adrenergic receptor blocking agents based on quantitative structure pharmacokinetic/pharmacodynamic relationship. Biol Pharm Bull. 1993; 16(12): 1251-1259.

Zhivcova Z and Doytchinova I. Prediction of steady-state volume of distribution of acidic drugs by quantitative structure–pharmacokinetics relationships. J Pharm Sci. 2012; 101: 1253-1266.